Explicit Temperature Treatment of Target Motion in Serpent 2

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Outline

- Introduction to the explicit temperature treatment method
- Current implementation in Serpent 2
- Howto?
- Test results for a HTGR system
- Future prospects
- Summary and conclusions

Explicit Temperature Treatment Method — Background

- Multi-physics applications of MC require detailed description of temperatures.
- When using conventional methods, the cross sections have to be stored in the computer memory separately for each nuclide and temperature.
  $\rightarrow$ Problem
- Solution: on-the-fly temperature treatment techniques [1].

[1] G. Yesilyurt, W. R. Martin and F. B. Brown, "On-the-fly Doppler Broadening for Monte Carlo Codes," *Proc. M&C 2009*, Saratoga Springs, New York, May 3–7 (2009).

Explicit Temperature Treatment Method — Background

- A new *stochastic* method for taking the thermal motion of target nuclei into account.
  - Introduced in NSE paper [2]
  - First practical results presented in PHYSOR 2012, Knoxville [3].
- Based on sampling the thermal motion of targets at collision sites and using 0 K cross sections in target-at-rest frame.

"There are no effective cross sections, only cross sections at 0 K and thermal motion of nuclei"

[2] T. Viitanen and J. Leppänen, "Explicit Treatment of Thermal Motion in Continous-energy Monte Carlo Tracking Routines," *Nuc. Sci. Eng.*, **171**, 165–173, (2012).

[3] T. Viitanen and J. Leppänen, "Explicit Temperature Treatment in Monte Carlo Neutron Tracking Routines – First Results." In Proc. PHYSOR-2012. Knoxville, TN, 15-20 April, 2012.

Explicit Temperature Treatment Method — Tracking scheme

1. Sample path length l based on a majorant cross section $\Sigma_{\text{maj}}(E)$
   $\rightarrow$ New collision point candidate $x_{i+1} = x_i + l$
2. Sample target nucleus n: $P_n = \frac{\Sigma_{\text{maj},n}(E)}{\Sigma_{\text{maj}}(E)} = \frac{\Sigma_{\text{maj},n}(E)}{\sum_n \Sigma_{\text{maj},n}(E)}$.
3. Sample target velocity from a Maxwellian-based distribution with $T = T(x_{i+1})$
   $\rightarrow$ Target-at-rest energy E'
4. Rejection sampling with criterion $\xi < \frac{g_n(E,T)\Sigma_{\text{tot},0\ \text{K},n}(E')}{\Sigma_{\text{maj},n}(E)}$
   - If the sample is rejected, return to 1.
   - If the sample is accepted, sample reaction using E' and zero-Kelvin cross sections. Continue accordingly.

Explicit Temperature Treatment Method — Calculating the Majorant

- The majorant for nuclide n is defined as

$$\Sigma_{\mathrm{maj}}(E) = g_n(E,T) \max_{E' \in [E-E_{\mathrm{t}},\ E+E_{\mathrm{t}}]} \Sigma_{\mathrm{tot,\ 0K}}(E')\,, \tag{1}$$

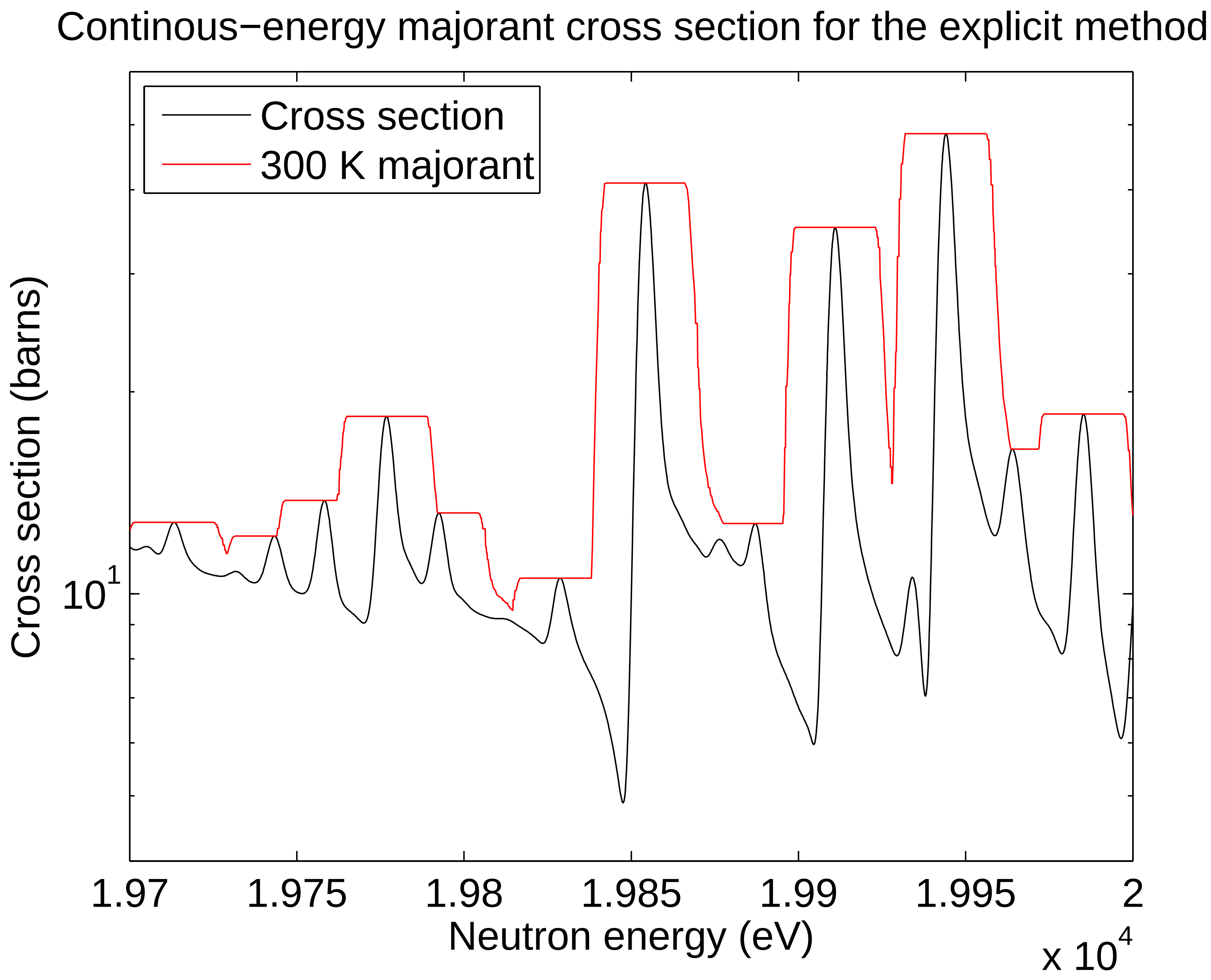
  where normalization factor $g_n(E,T)$ accounts for the increase in potential scattering at low energies.

- Cut-off $E_t < 16kT/A_n$ is utilized for the kinetic energy of the target nucleus E_t [4, 5].

- In case the temperature within a material is inhomogeneous, a maximum temperature $T = T_{\mathrm{max}}$ is used when generating the majorant.

[4] D. E. Cullen, "Program SIGMA1 (version 79-1): Doppler broaden evaluated cross sections in the evaluated nuclear data file/version B (ENDF/B) format," UCRL-50400 Part B., Lawrence Livermore National Laboratory (1979).

[5] B. Becker, R. Dagan and G. Lohnert, "Proof and implementation of the stochastic formula for ideal gas, energy dependent scattering kernel," *Ann. Nucl. Energy*, **36**, pp. 470–474 (2009).



Continous−energy majorant cross section for the explicit method
Cross section
300 K majorant
Cross section (barns)
10^1
1.97
1.975
1.98
1.985
1.99
1.995
2
Neutron energy (eV)
x 10^4

Explicit Temperature Treatment Method — Sampling the target velocity

- Target velocity V_t is sampled from $f(V_{\mathrm{t}}, \mu) = \frac{v'}{2v} f_{\mathrm{MB}}(V_{\mathrm{t}})$ where $f_{\mathrm{MB}}(V_{\mathrm{t}}) = \frac{4}{\sqrt{\pi}} \gamma^3 V_{\mathrm{t}}^2 e^{-\gamma^2 V_{\mathrm{t}}^2}$ is the Maxwell-Boltzmann distribution.
- The same distribution and, hence, the same sampling procedure as in the standard free gas treatment [6].

[6] MCNP X-5 Monte Carlo Team, “MCNP — a General Monte Carlo N-Particle Transport Code,” Version 5, LA-UR-03-1987, Los Alamos National Laboratory (2003).

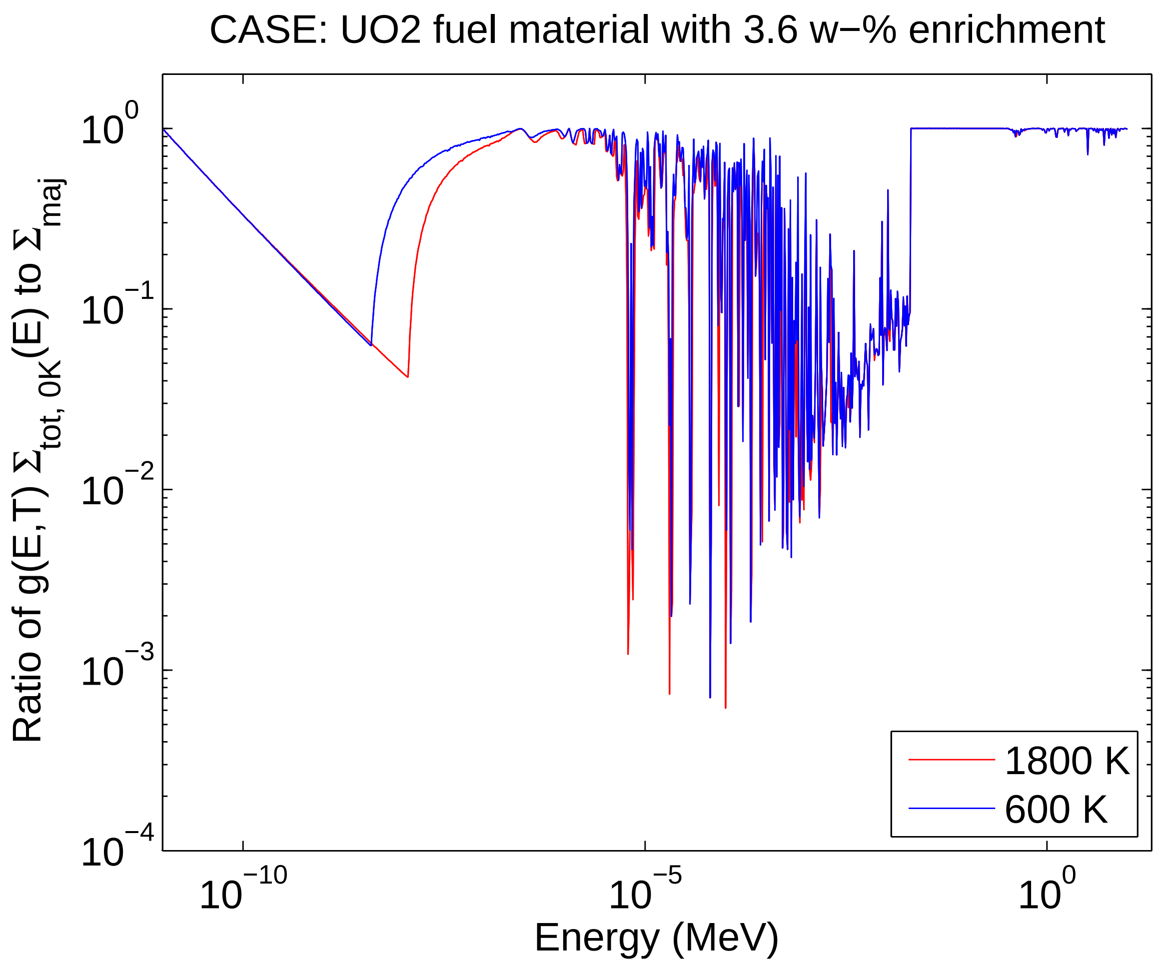
Explicit Temperature Treatment Method — Properties

- Only 0 Kelvin cross sections are needed during tracking $\rightarrow$ Memory consumption does not depend on the number of temperatures in the problem geometry.
- Inhomogeneous temperatures *are* allowed within a material zone, i.e. temperature distribution can be modelled with an arbitrary function $T = T(x)$
- The sampled target velocities can be recycled when calculating kinematics of scattering events.
  - Inherently correct secondary particle distributions!
- Track-length estimators cannot be used for reaction rates.

Preliminary implementation in Serpent 2

- Multi-group majorant cross sections with 40 000 equi-lethargy energy groups.
  - Fast calculation of Σ_{maj}
  - Reduced memory consumption per nuclide compared to continous-energy implementation.
  - Reduced sampling efficiency during transport.
    $\xi < \frac{g_n(E,T)\Sigma_{\mathrm{tot},0\ \mathrm{K},n}(E')}{\Sigma_{\mathrm{maj},n}(E)}$
- Reaction rate estimators not yet implemented. Hence, only flux spectrum and k_{eff} can be calculated.

A few words about the efficiency of the method



Usage of the on-the-fly method

- In Serpent 2, on-the-fly temperature treatment can be activated with input card

```
set dop 2
```

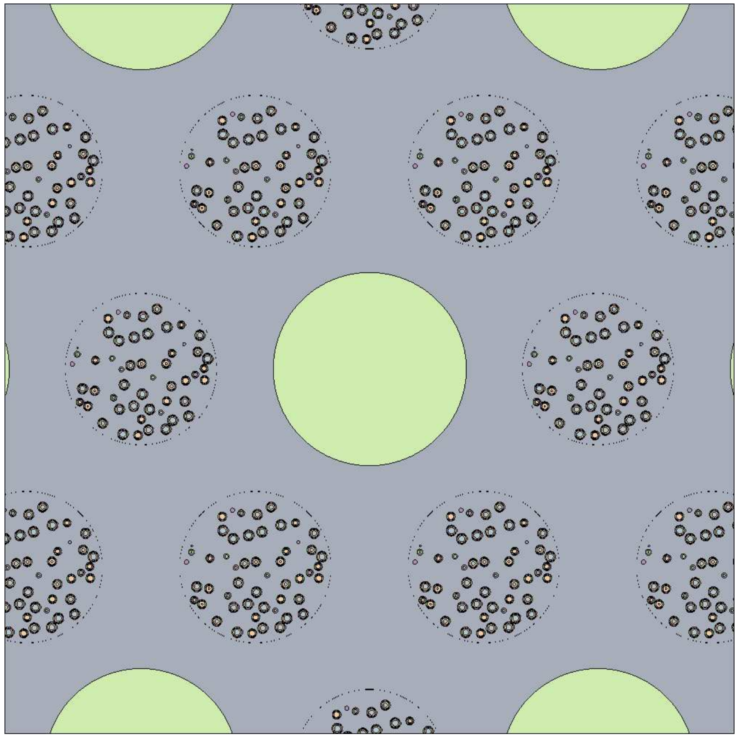
- When activated, the explicit temperature treatment is used for all materials with a tmp card.
  - Cross sections for these materials must be at 0 K.

- IMPORTANT! The explicit treatment cannot be used for materials containing bound scatterers.

```
mat fuel -10.4 tmp 900
92235.00c   -0.03173
92238.00c   -0.84977
 8016.00c   -0.11850
```

HTGR test case

- A HTGR system consisting of 6 compacts in a graphite matrix surrounding a coolant channel full of helium. Fuel is at 1800 K, other solid materials are at 1200 K and helium is at 900 K temperature.



Results — HTGR system

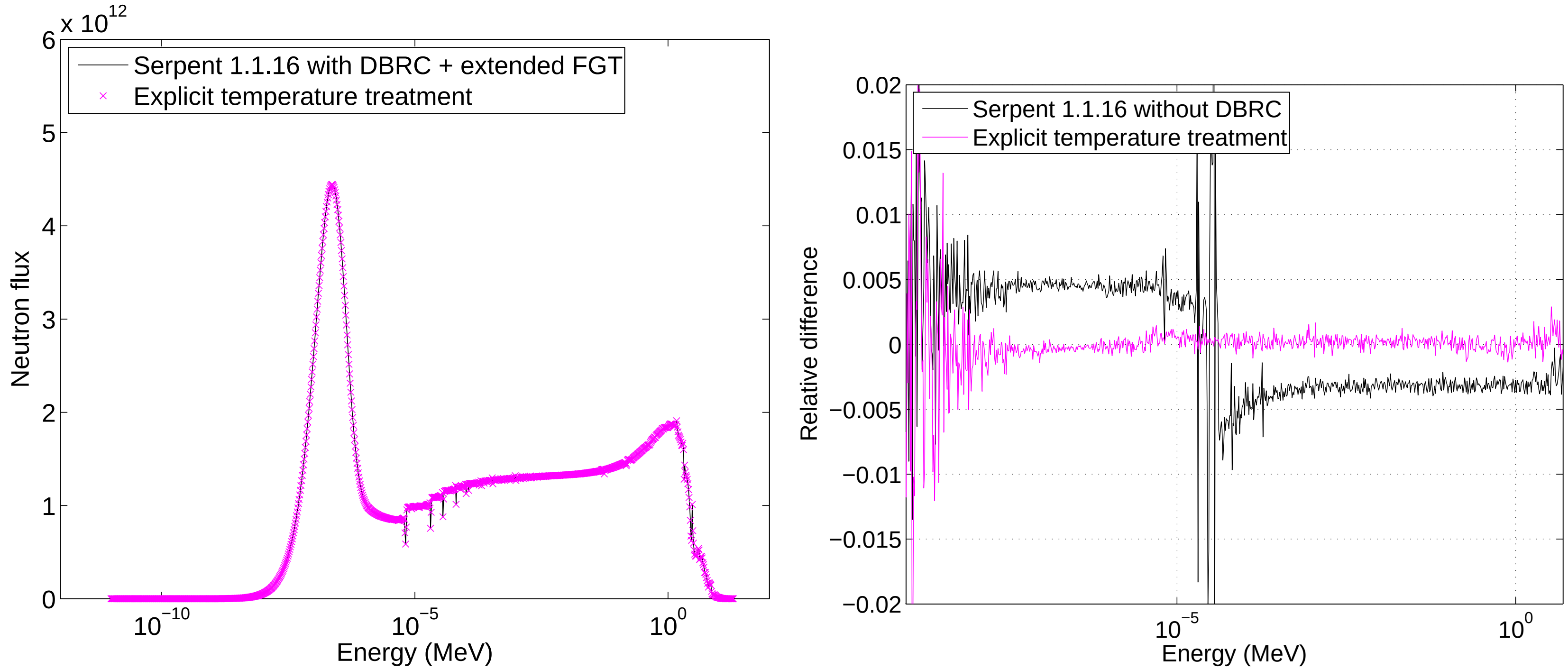


Figure 1: **Left:** Neutron flux normalized to 1E15 total flux. **Right:** Difference to a benchmark calculated using Serpent 1.1.16 with NJOY-broadened cross sections and DBRC.

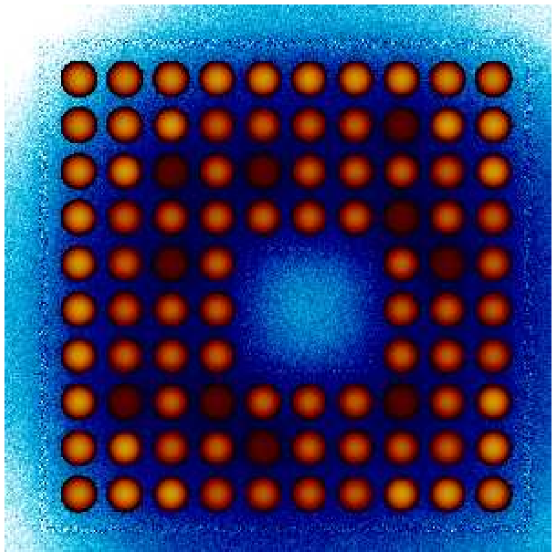
Results — Performance

Table 1: **Total CPU times of the simulations.**

HTGR			PWR pin-cell		
Case	Time (s)	Ratio	Case	Time (s)	Ratio
Serpent 2, explicit	3497.0	**4.20**	Serpent 2, explicit	1585.4	**2.28**
Serpent 2, optimiz. mode 2	830.9	1.00	Serpent 2, optimiz. mode 2	696.3	1.00
Serpent 1.1.16+DBRC+FGT	911.7	1.10	Serpent 1.1.16+DBRC	463.0	0.66
Serpent 1.1.16	845.6	1.02	Serpent 1.1.16	425.9	0.61

Future Prospects

- Extension of the method to the unresolved region and bound-atom scattering.
- Optimization of the implementation.
- Implementation of reaction rate estimators.
- Burnup calculation in otf mode.
- Application: a built-in thermal feedback calculator for pin geometries (M.Sc. project of V.Valtavirta, Aalto University).



Summary and conclusions

- A new stochastic method for taking the thermal motion of target nuclei into account has been developed and preliminarily implemented in Serpent 2.
- With the new method, temperatures can be modelled with an arbitrary function $T(x)$, independent of material boundaries.
- Transport with the current implementation requires about 2–4 times more CPU time than with traditional methods, depending on the case.
- Extension of the method to bound-atom scattering and unresolved energy range requires further work.

References

[1] G. Yesilyurt, W. R. Martin and F. B. Brown, “On-the-fly Doppler Broadening for Monte Carlo Codes,” *Proc. M&C 2009*, Saratoga Springs, New York, May 3–7 (2009).

[2] T. Viitanen and J. Leppänen, “Explicit Treatment of Thermal Motion in Continous-energy Monte Carlo Tracking Routines,” *Nuc. Sci. Eng.*, **171**, 165–173, (2012).

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